5th JCS International Symposium on Theoretical Chemistry

December 2-6, 2013

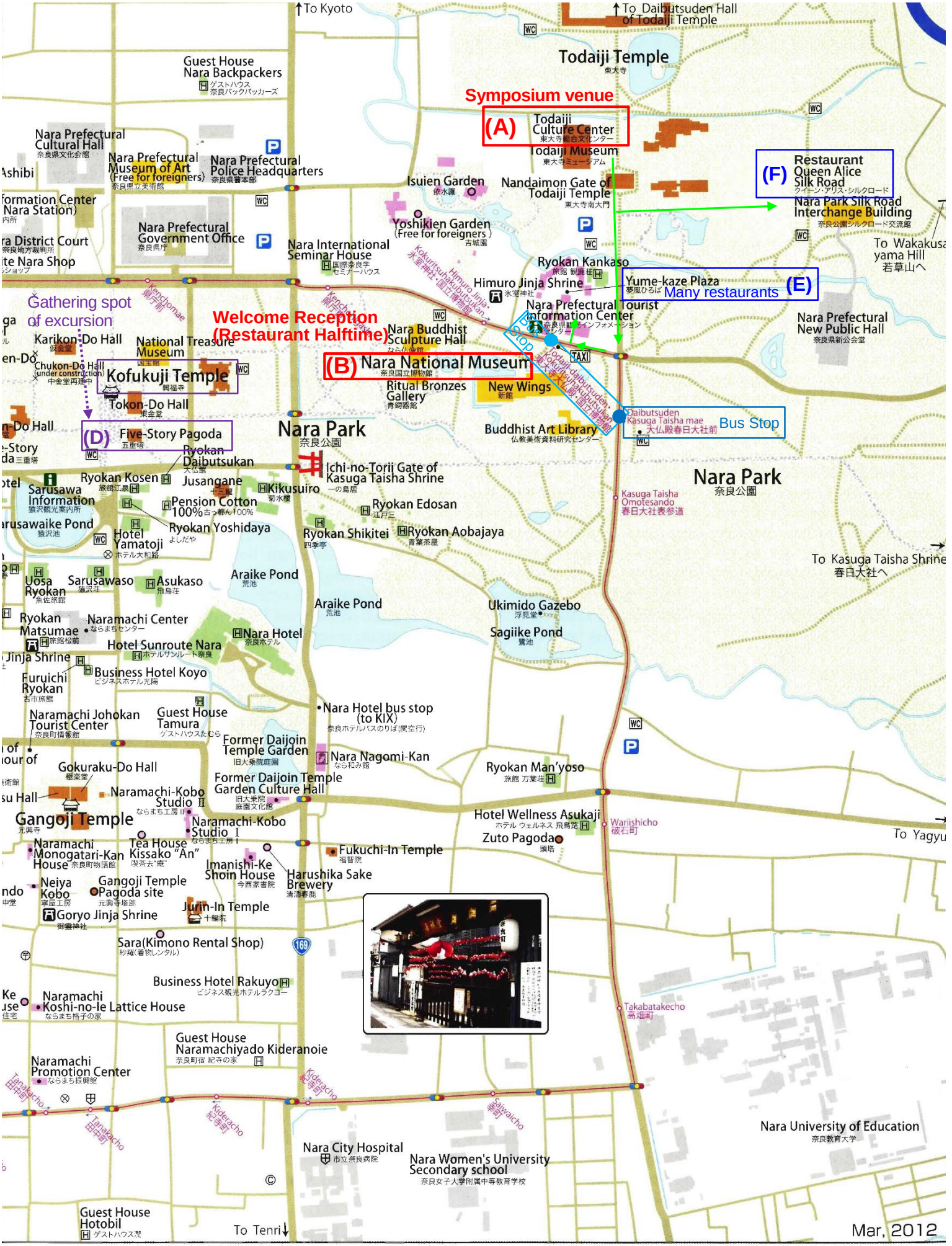
Todai-ji Culture Center, Nara, Japan

5th JCS International Symposium Map

Nara Prefectural Tourist Information Center
奈良県観光インフォメーションセンター（奥村記念館内）
(10:00～17:00) TEL.0742-27-2003

Nara City Tourist Information Center
Nara City Tourist Information Center (Next to JR Nara Station)
奈良市総合観光案内所 (9:00～21:00) TEL.0742-27-2223
※Left Luggage 一時荷物預り

JR Nara Station ＪＲ奈
Nara City Tourist Cer
奈良市観光センター (9:00



良駅総合観光案内所 (9:00～17:00)
ter (Sanjodori Street)
～21:00) TEL.0742-22-5595

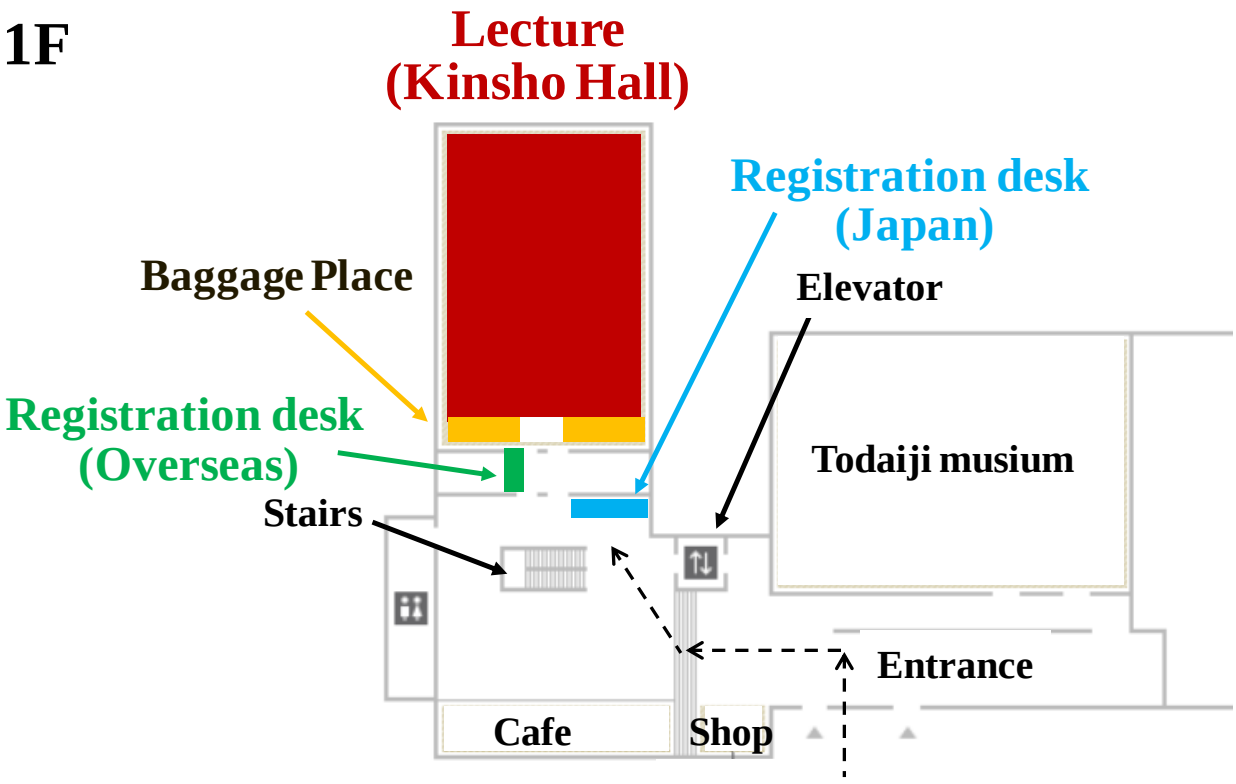
Kintetsu-Nara Station
近鉄奈良駅総合観光案内所 (9:00～17:00) TEL.0742-24-4858
Sarusawa Information 猿沢観光案内所 (9:00～17:00)

Free Tours in English

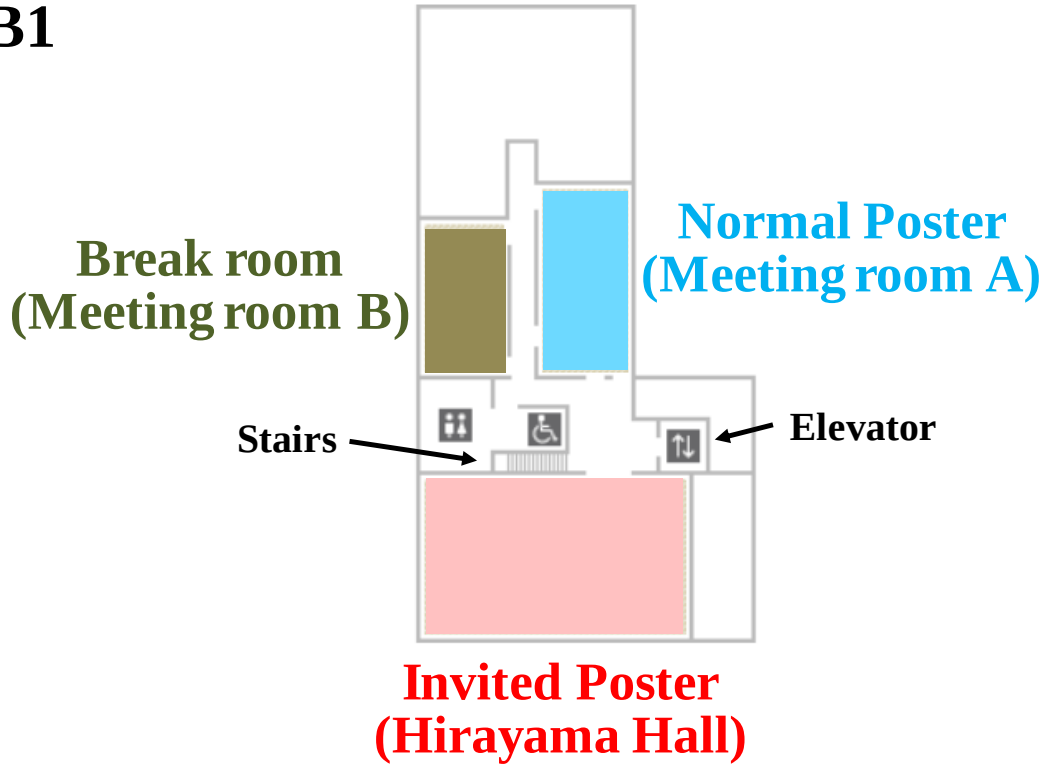
Nara S.G.G.Club TEL.0742-22-5595 FAX.0742-22-5595
Nara Student Guide TEL.0742-26-4753 FAX.0742-26-1991
Nara YMCA Goodwill Guides TEL.0742-45-5920

Floor guide (Todai-ji Culture Center)

1F



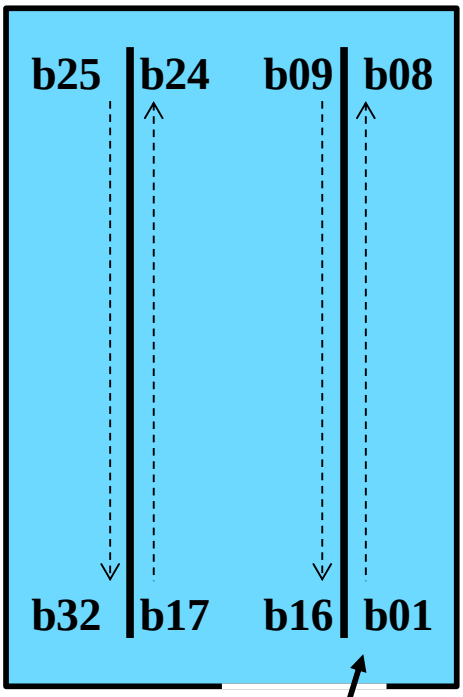
B1



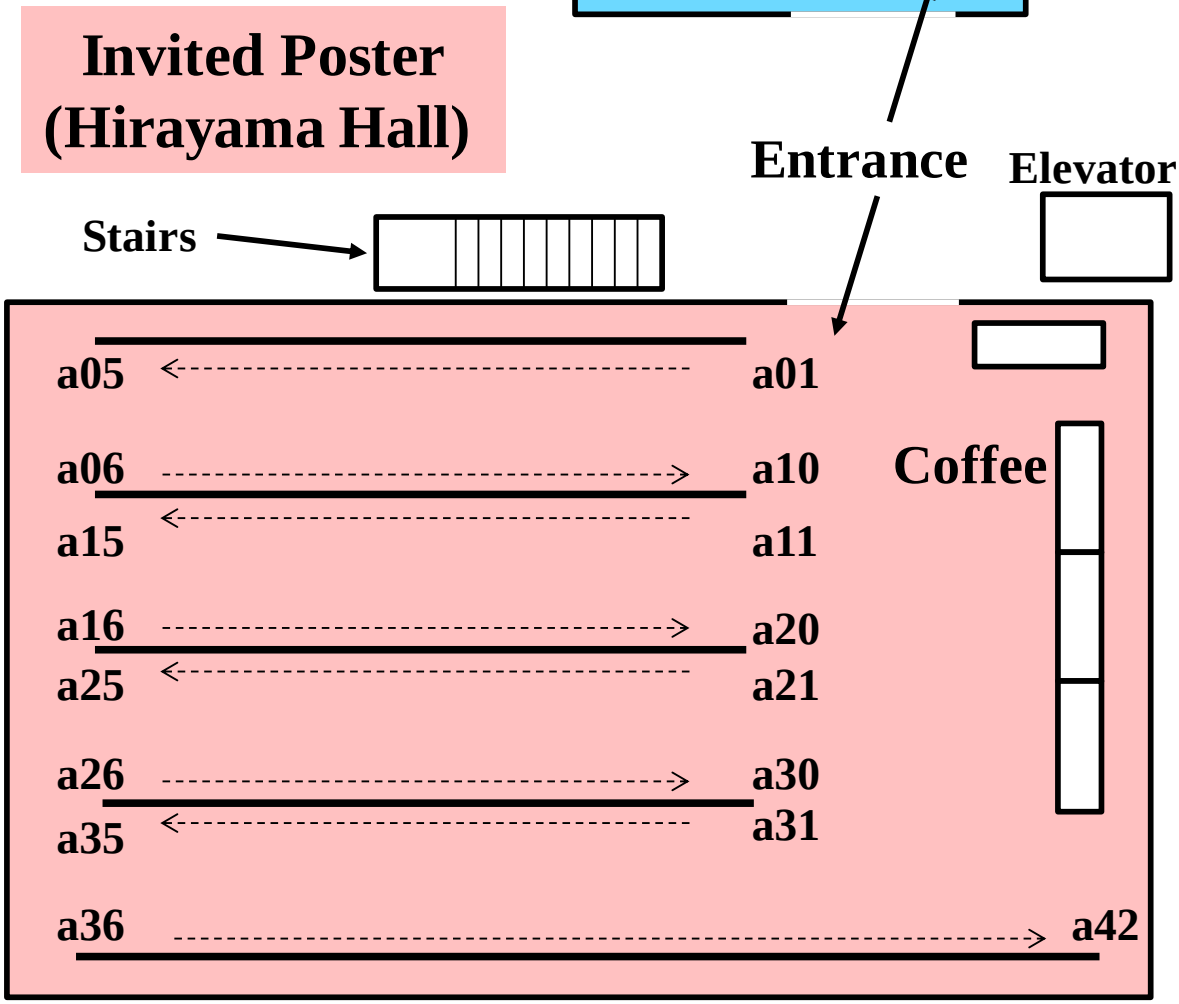
Poster session

B1

Normal Poster (Meeting room A)



Invited Poster (Hirayama Hall)



Locations

Symposium venue: Todai-ji Culture Center (Map A)

Todai-ji Culture Center is located close to **NanDaiMon (South Big Gate)** of Todai-ji Temple, which is one of the most historical temples (registered as a UNESCO World Heritage) and famous with its Big Buddha. Todai-ji is a Buddhism temple but the venue is free from the religions. The place around the venue is very peaceful and nice for sightseeing.

Welcome reception: Halftime (Map B)

Place: Restaurant Halftime (葉風泰夢) located B1 of Nara National Museum
7 minutes' walk from the symposium venue
Date: Dec 2, 18:30-20:30

Banquet: Hotel Nikko Nara (Map C)

Place: Hotel Nikko Nara, room Hiten (飛天) (4F)
Date: Dec 5, 19:00-21:00
Hotel Nikko Nara locates just next to the JR Nara station.

Excursion

Date: Dec 6, 9:00-16:00

Gathering spots (Map C or D):

The starting spot is Hotel Nikko Nara. But if it is convenient for you, you can join from Kofukuji Temple. Our staffs will be waiting at both places.

Please gather either **at the lobby of Hotel Nikko Nara at 8:50 (Map C)** or **in front of Five-Story Pagoda in Kofukuji Temple at 9:20 (Map D)**. "Kofukuji" is often written as "Kohfukuji" or "Koufukuji".

Lunch

Yume-Kaze Plaza (Map E)

There are more than ten restaurants and shops in this plaza.

Restaurant Halftime (Map B)

B1 in Nara National Museum. Chinese food, curry and rise, noodles, etc. are served.

Welcome reception is held here.

Restaurant Queen Alice Silkroad (Map F)

It locates in Nara Park.

There are also other restaurants but there is no convenience store around the conference venue.

Dinner

There are many restaurants around Kintetsu Nara station (Map G).

Please enjoy Japanese-style bar ("Izakaya" in Japanese) and wine bar etc.

Important notes and information

Oral presentation

Official language: English

Total time for one oral presentation: 20 min
0 - 15 min: Presentation (Color of Timer: Green (0-12 min) and Yellow (12-15 min))
15 - 19 min: Discussion (Color of Timer: Orange)
19 min: Finish (Color of Timer: Red)
19 - 20 min: PC connection etc.
(Timer system is displayed near the speaker.)

Be sure to check your PC connection before your lecture in coffee break, lunch time etc.

Poster presentation

Place and Space
Invited Poster : Hirayama Hall, A0×2 space
Normal Poster: Meeting Room A, A0 space

Poster I (Dec 3, 15:00 - 16:40)
Please put up the posters from 12:00 on Dec 2.
Please take off the posters promptly after the end of the presentation.

Poster II (Dec 4, 15:00 - 16:40)
Please put up the poster from 9:00 on Dec 4.
Please take off the poster by the end of the last coffee break (15:40 on Dec 5.).

Registration desk

Registration desk open: Dec 2, 12:00-

Food or drinks in the symposium venue

No food or drinks allowed inside "Kinsho Hall" (Lecture room): very strict
Hirayama hall and Break room in B1 floor are allowed to drink coffee, tea, etc. but no foods.
Drinking alcohol in the symposium venue is strictly prohibited because the venue is located in the Buddhism Temple, Todai-ji.

Internet

Wireless internet access is available in "Kinsho Hall" (Lecture room)

Transportation

From Kansai-airport

(1) Recommend: Kansai Airport - (Limousin Bus: 90 minutes) - JR Nara station
More information, http://www.kate.co.jp/pc/e_time_table/e_nara.html

(2) Kansai Airport - (JR Kansai-kuukou(airport) Line: 30 minutes) - Tennoji - (JR Kaisoku Yamatoji Line: 30 minutes) - JR Nara station

(3) Kansai Airport - (Nankai Line: 30 minutes) - Namba - (Kintetsu Nara Line: 30 minutes) - Kintetsu Nara station

From Narita-airport

Narita Airport - (JR Narita Express: 60 minutes) - JR Tokyo station - (JR Shinkansen Super Express: 150 minutes) - JR Kyoto station - Kintetsu Kyoto station - (Kintetsu Kyoto Line: 40 minutes (Limited express), 50 minutes (Express)) - Kintetsu Nara station

From Osaka City

(1) Kintetsu Namba - (Kintetsu Nara Line: 30 minutes) - Kintetsu Nara station

(2) JR Osaka station - (JR Kaisoku Yamatoji Line: 50 minutes) - JR Nara station

From Kyoto City

(1) Kintetsu Kyoto station - (Kintetsu Kyoto Line: 40 minutes (Limited express), 50 minutes (Express)) - Kintetsu Nara station

(2) JR Kyoto station - (JR Nara Line: 60 minutes) - JR Nara station

Emergency

In case of medical emergencies, dial 119, and police, dial 110.
Cell phone: Hiroshi Nakatsuji 090-1028-7250, Hiroyuki Nakashima 090-8468-8047
Contact Registration Desk

Organizing committee of the 5th JCS international symposium on theoretical chemistry

International organizer

Chair: Hiroshi Nakatsuji	Quantum Chemistry Research Institute (Japan)
Vice-Chair: Masahiro Ehara	Institute of Molecular Science (Japan)
Zdeněk Havlas	Institute of Chemistry and Biochemistry, Academy of Science of the Czech Republic (Czech Republic)
Lubomír Rulíšek	Institute of Chemistry and Biochemistry, Academy of Science of the Czech Republic (Czech Republic)
Petr Čársky	J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic (Czech Republic)
Jiří Pittner	J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic (Czech Republic)
Miroslav Urban	Comenius University (Slovak Republic)
Vladimir Kellö	Comenius University (Slovak Republic)

Local organizer

Chair: Hiroyuki Nakashima	Quantum Chemistry Research Institute (Japan)
Vice-Chair: Tomoo Miyahara	Quantum Chemistry Research Institute (Japan)
Vice-Chair: Yusaku I. Kurokawa	Quantum Chemistry Research Institute (Japan)

5th JCS International Symposium on Theoretical Chemistry

– Program –

December 2-6, 2013

Todai-ji Culture Center, Nara, Japan

Welcome to the 5th JCS International Symposium on Theoretical Chemistry

Profs. R. Zahradnik, Z. Havlas, and H. Nakatsuji initiated the JCS symposium on theoretical chemistry in 2004 based on the high-level scientific relationship and warm friendship between Japanese and Czech theoretical chemists. Slovak theoretical chemists joined in 2006. Four previous symposia were held at IOBC in Praha (2005), Fukui Institute in Kyoto (2007), Comenius University in Bratislava (2009), Chateau Liblice in Praha (2011).

The 5th Symposium is now held at the Todai-ji Culture Center of Todaiji Temple in Dec 2-6, 2013. In this symposium, we slightly expanded the participating countries more than three (JCS + I) with our basic organizing policy; "Friendship is our principle, Science will follow with us". The objective of this symposium is to deepen our friendship, ideas, and understandings on our science, culture, and life, and then create new science and develop peaceful world. Actually, several international collaborative studies have started through the previous JCS symposia. In the present symposium, Poster Session is also a Key Session, in addition to the invited lecture session: we initiated Invited Poster in addition to the normal one to activate fruitful discussions among the attendants of this symposium.

Nara was a capital of our country for 710 - 784 with an intermission of five years. The symposium venue (Todai-ji Culture Center) is located close to the Nan-Dai-Mon (South Big Gate) of To-Dai-Ji (East Big Temple), which is one of the most historical temples in our country and famous with its Big Buddha. It is registered as a UNESCO World Heritage. Todai-ji is a Buddhism temple but the venue is free from the religion. The place around the venue is very peaceful and nice for sightseeing.

Please enjoy, not only science but also historical Nara, together with the talks with your friends on science culture, and life during the symposium.

Chair of the 5th JCSI symposium organizers,
International, Hiroshi Nakatsuji,
Local, Hiroyuki Nakashima

Scientific Program

Dec 2 (Monday)	Dec 3 (Tuesday)	Dec 4 (Wednesday)	Dec 5 (Thursday)	Dec 6 (Friday)
	8:30-10:10 **Invited Lecture c** (Chair: Hiroshi Nakatsuji) Petr Čárský Yuki Kurashige Lubomír Rulíšek Haruki Nakamura Akihiro Morita	**8:30-10:10** **Invited Lecture g** (Chair: Satoshi Yabushita) Satoshi Maeda Jiří Pittner Shinkoh Nanbu Tetsuya Taketsugu Susumu Okazaki	**8:30-10:10** **Invited Lecture k** (Chair: Tomoo Miyahara) Lubomír Skála Akitomo Tachibana Mojmir Kývala Koji Ando Ján Urban	**9:00-16:00** **Excursion**
	Coffee Break (40 min.)	**Coffee Break (40 min.)**	**Coffee Break (40 min.)**	
	10:50-12:10 **Invited Lecture d** (Chair: Takeshi Yanai) Jun-ya Hasegawa Kaori Fukuzawa Shozo Yanagida Pavel Hobza	**10:50-12:10** **Invited Lecture h** (Chair: Hisashi Okumura) Henryk Witek Tomáš Bučko Hirohiko Kono Takeshi Sato	**10:50-12:10** **Invited Lecture l** (Chair: Yusaku Kurokawa) Takefumi Yamashita Petr Slavíček Susumu Yanagisawa Petr Jurečka	
12:00- **Registration**	**Take Photo**	**12:10-13:40** **Lunch (90 min.)**	**12:10-13:40** **Lunch (90 min.)**	
	12:10-13:40 **Lunch (90 min.)**			
14:00-14:10 **Opening Address** Hiroshi Nakatsuji	**13:40-15:00** **Invited Lecture e** (Chair: Hiroyuki Nakashima) Misako Aida Kazunobu Sato Vladimír Malkin Olga Malkina	**13:40-15:00** **Invited Lecture i** (Chair: Manabu Sugimoto) Yoshitada Morikawa Michal Straka Nurbosyn U. Zhanpeisov Vladimír Špirko	**13:40-15:00** **Invited Lecture m** (Chair: Susumu Kawauchi) Jan Rezac Yoong-Kee Choe Pavel Banáš Hajime Torii	
14:10-15:30 **Opening Lecture a** (Chair: Masahiro Ehara) Zdeněk Havlas Keiji Morokuma Miroslav Urban Shigeyoshi Sakaki	**15:00-16:40** **Poster I** **(B1: Hirayama Hall and Meeting Room A)**	**15:00-16:40** **Poster II** **(B1: Hirayama Hall and Meeting Room A)**	**Coffee Break (40 min.)**	
Coffee Break (60 min.)			**15:40-17:20** **Invited Lecture n** (Chair: Suehiro Iwata) Masayoshi Takayanagi Martin Srnec Mitsutaka Okumura Masahiko Hada (changed from Jaroslav Burda) Kazunari Yoshizawa	
16:30-17:50 **Opening Lecture b** (Chair: Masahiko Hada) Josef Michl Kazuo Kitaura Wieslaw Nowak Koichi Yamashita	**16:40-18:00** **Invited Lecture f** (Chair: Ryoichi Fukuda) Masato Kobayashi Nobuaki Koga Lukáš Bučinský Masayoshi Nakano	**16:40-18:00** **Invited Lecture j** (Chair: Yasuteru Shigeta) Stanislav Záliš Ivana Paidarová Masanori Tachikawa Ivan Štich		
18:30-20:30 **Welcome Reception** **(Restaurant Halftime, B1 of Nara National Museum)**			**19:00-21:00** **Banquet** **(Hotel Nikko Nara, 4F, Room Hiten)**	

Monday, Dec 2

12:00- **Registration**

14:00-14:10 **Opening**

14:00 **Hiroshi Nakatsuji**
Quantum Chemistry Research Institute
"Opening Address – Welcome!"

14:10-15:30 **Opening Lecture a** (Chair: Masahiro Ehara)

14:10 Oa-1 **Zdeněk Havlas**
Institute of Chemistry and Biochemistry, Academy of Science of the Czech Republic
"Modeling dimer structure for efficient singlet fission"

14:30 Oa-2 **Keiji Morokuma**
Fukui Institute for Fundamental Chemistry, Kyoto University, Japan
"Complex Chemical Reaction Pathways Explored by Automatic Search Strategy"

14:50 Oa-3 **Miroslav Urban**
Comenius University, Slovak Republic
"Toward understanding the bonding character and electric properties of coinage metals - lone pair ligands complexes"

15:10 Oa-4 **Shigeyoshi Sakaki**
Fukui Institute for Fundamental Chemistry, Kyoto University, Japan
"Gas Absorption and Spin Transition of the Hofmann-type Metal Organic Framework: Theoretical Study"

15:30-16:30 **Coffee Break**

16:30-17:50 **Opening Lecture b** (Chair: Masahiko Hada)

16:30 Ob-1 **Josef Michl**
Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
"Computational Modeling of Inclusion Compounds Containing Dipolar Molecular Rotors"

16:50 Ob-2 **Kazuo Kitaura**
Kobe University, Japan
"Analytic Second Derivatives in the Fragment Molecular Orbital Method"

17:10 Ob-3 **Wieslaw Nowak**
Nicolaus Copernicus University, Poland
"Theoretical Approach to Nanomechanics of Modular Proteins"

17:30 Ob-4 **Koichi Yamashita**
The University of Tokyo, Japan
"First-Principles Calculations on Switching Mechanism of a Molecule on Metal Surfaces"

18:30-20:30 **Welcome Reception (Restaurant Halftime (葉風泰夢), B1 of Nara National Museum)**

Tuesday, Dec 3

8:30-10:10 **Invited Lecture c** (Chair: Hiroshi Nakatsuji)

8:30 Oc-1 **Petr Čársk**ý
J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic
"Evaluation of exchange integrals by Fourier transform of the 1/r operator and its numerical quadrature (Prospects for treatments of large molecules by methods giving results more accurate than the present DFT)"

8:50 Oc-2 **Yuki Kurashige**
Institute for Molecular Science, Japan
"Entangled quantum electronic wavefunctions of the Mn_4CaO_5 cluster in photosystem II"

9:10 Oc-3 **Lubomír Rulíšek**
Institute of Organic Chemistry and Biochemistry, Gilead Sciences & IOCB Research Center, Academy of Sciences of the Czech Republic
"DMRG-CASPT2 and DFT Studies on Reactive Intermediates in Non-Heme Diiron Enzymes"

9:30 Oc-4 **Haruki Nakamura**
Osaka University, Japan
"Towards Quantitative Analysis and Prediction of Protein-Protein Interactions"

9:50 Oc-5 **Akihiro Morita**
Tohoku University, Japan
"Molecular Science for Liquid Interfaces"

10:10-10:50 Coffee Break

10:50-12:10 Invited Lecture d (Chair: Takeshi Yanai)

10:50 Od-1 **Jun-ya Hasegawa**
Hokkaido University, Japan
"Molecular Excited States in Proteins and Solutions"

11:10 Od-2 **Kaori Fukuzawa**
Mizuho Information & Research Institute, Inc., Japan
"Fragment Molecular Orbital Study for Biomolecular Systems"

11:30 Od-3 **Shozo Yanagida**
Osaka University, Japan
"Computer-chemistry understandings on worldwide anxious chemical reactions"

11:50 Od-4 **Pavel Hobza**
Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
"How accurate are "gold standard" CCSD(T)/CBS interaction energies?"

12:10 Take Photo

12:10-13:40 Lunch

13:40-15:00 Invited Lecture e (Chair: Hiroyuki Nakashima)

13:40 Oe-1 **Misako Aida**
Hiroshima University, Japan
"Helmholtz Energy Change between Neutral and Zwitterionic Forms of Glycine in Aqueous Solution"

14:00 Oe-2 **Kazunobu Sato**
Osaka City University, Japan
"Organic Open-Shell Systems as Models for Molecular Spin Quantum Computers and Spin Manipulation by Pulsed ESR Technology"

14:20 Oe-3 **Vladimír Malkin**
Institute of Inorganic Chemistry, Slovak Academy of Sciences, Slovak Republic
"Four-Component Relativistic DFT Calculations of NMR Shielding Tensors for Paramagnetic Systems"

14:40 Oe-4 **Olga Malkina**
Institute of Inorganic Chemistry, Slovak Academy of Sciences, Slovak Republic
"Recent progress in relativistic four-component calculations in NMR indirect nuclear spin-spin coupling constants"

15:00-16:40 Poster I (B1: Hirayama Hall and Meeting Room A)

16:40-18:00 Invited Lecture f (Chair: Ryoichi Fukuda)

16:40 Of-1 **Masato Kobayashi**
Waseda University, Japan
"Divide-and-conquer method for linear-scaling electronic structure calculations"

17:00 Of-2 **Nobuaki Koga**
Nagoya University,Japan
"Theoretical Study of Reactions of Nitriles with Organotransition Metal Complexes"

17:20 Of-3 **Lukáš Bučinský**
Slovak University of Technology, Slovak Republic
"Relativistic effects in the topology of electron density and properties of 2-component spin densities"

17:40 Of-4 **Masayoshi Nakano**
Osaka University, Japan
"Theoretical Study on the Optical Properties of Open-Shell Singlet Molecular Systems"

Wednesday, Dec 4

8:30-10:10 **Invited Lecture g** (Chair: Satoshi Yabushita)

8:30 Og-1 **Satoshi Maeda**
Hokkaido University, Japan
"Systematic Exploration of Transition State Structures for Organic Reactions by the Artificial Force Induced Reaction (AFIR) Method"

8:50 Og-2 **Jiří Pittner**
J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic
"Molecular dynamics with non-adiabatic and spin-orbit effects"

9:10 Og-3 **Shinkoh Nanbu**
Sophia University, Japan
"*Ab Initio SemiClassical Molecular Dynamics (AI-SCMD) of nonadiabatic photochemical reaction*"

9:30 Og-4 **Tetsuya Taketsugu**
Hokkaido University, Japan
"Ab initio Molecular Dynamics Approach to Tunneling Splitting Calculations"

9:50 Og-5 **Susumu Okazaki**
Nagoya University, Japan
"An all-atomistic molecular dynamics calculation study of virus using K-computer"

10:10-10:50 **Coffee Break**

10:50-12:10 **Invited Lecture h** (Chair: Hisashi Okumura)

10:50 Oh-1 **Henryk Witek**
National Chiao Tung University, Taiwan
"Structure of Analytical Wave Function of Helium Atom"

11:10 Oh-2 **Tomáš Bučko**
Comenius University, Slovak Republic
"Improved Density Dependent Correction for the description of London Dispersion Forces"

11:30 Oh-3 **Hirohiko Kono**
Tohoku University, Japan
"Characterization of Multielectron Dynamics in Molecules: A Multiconfiguration Time-dependent Hartree-Fock Picture"

11:50 Oh-4 **Takeshi Sato**
The University of Tokyo, Japan
"Time-dependent MCSCF methods for multielectron dynamics in intense laser fields"

12:10-13:40 **Lunch**

13:40-15:00 **Invited Lecture i** (Chair: Manabu Sugimoto)

13:40 Oi-1 **Yoshitada Morikawa**
Osaka University, Japan
"First-principles simulations of chemical reactions at interfaces"

14:00 Oi-2 **Michal Straka**
Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
"Theoretical calculations of ^{129}Xe NMR parameters"

14:20 Oi-3 **Nurbosyn U. Zhanpeisov**
Tohoku University, Japan
"Theoretical DFT Study on New Carbon K4 and Metal-Organic Framework Structures"

14:40 Oi-4 **Vladimír Špirko**
Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
"Localised Quantum States of Atomic and Molecular Particles Physisorbed on Carbon-Based Nanoparticles"

15:00-16:40 **Poster II (B1: Hirayama Hall and Meeting Room A)**

16:40-18:00 **Invited Lecture j** (Chair: Yasuteru Shigeta)

16:40 Oj-1 **Stanislav Záliš**
J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic
"Spin Orbit Effects in Re and Pt Organometallic Complexes"

17:00 Oj-2 **Ivana Paidarová**
J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic
"Towards theoretical description of state-selected reactions of O^+ with methane"

17:20 Oj-3 **Masanori Tachikawa**
Yokohama City University, Japan
"First-principles calculation for positron binding to molecules"

17:40 Oj-4 **Ivan Štich**
Institute of Physics, Slovak Academy of Sciences, Slovak Republic
"Magnetism and spin transport in transition metal organometallic molecules"

Thursday, Dec 5

8:30-10:10 **Invited Lecture k** (Chair: Tomoo Miyahara)

8:30 Ok-1 **Lubomír Skála**
Charles University, Czech Republic
"Internal structure of the Heisenberg and Robertson-Schrödinger uncertainty relations"

8:50 Ok-2 **Akitomo Tachibana**
Kyoto University, Japan
"Time evolution of quantum system based on QED: Formulation and Simulation"

9:10 Ok-3 **Mojmir Kývala**
Institute of Organic Chemistry and Biochemistry, Czech Republic
"Search for a molecule with a measurable electronic energy shift due to parity violation"

9:30 Ok-4 **Koji Ando**
Kyoto University, Japan
"Electron and nuclear wave packet modeling of chemical bonding and dynamics"

9:50 Ok-5 **Ján Urban**
Comenius University, Slovak Republic
"Fragmentation of Negative Ions - Theoretical Description"

10:10-10:50 **Coffee Break**

10:50-12:10 **Invited Lecture *l*** (Chair: Yusaku Kurokawa)

10:50 O*l*-1 **Takefumi Yamashita**
The University of Tokyo, Japan
"Proton transport in biomolecular and aqueous systems: A molecular dynamics approach"

11:10 O*l*-2 **Petr Slavíček**
Institute of Chemical Technology and J. Heyrovský Institute of Physical Chemistry, Czech Republic
"New Ultrafast Relaxation Processes in Hydrogen Bonded Systems"

11:30 O*l*-3 **Susumu Yanagisawa**
University of the Ryukyus, Japan
"Intermolecular interaction as origin of red shifts in absorption spectra of Zinc-Phthalocyanine from first-principles"

11:50 O*l*-4 **Petr Jurečka**
Palacký University, Czech Republic
"Force Field Refinements for RNA and DNA Simulations Derived from Accurate QM Calculations with Inclusion of Solvation Effects"

12:10-13:40 **Lunch**

13:40-15:00 **Invited Lecture m** (Chair: Susumu Kawauchi)

13:40 Om-1 **Jan Rezac**
Institute of Organic Chemistry and Biochemistry, Academy of Science of the Czech Republic
"Benchmark databases and method development in the Cuby framework"

14:00 Om-2 **Yoong-Kee Choe**
National Institute of Advanced Industrial Science and Technology, Japan
"Nature of proton transport in polymer electrolyte membranes for fuel cell applications"

14:20 Om-3 **Pavel Banáš**
Palacký University, Czech Republic
"RNA catalyzes: An Insight from molecular dynamics simulations and QM/MM calculations"

14:40 Om-4 **Hajime Torii**
Shizuoka University, Japan
"The Role of Delocalized Electrons in Infrared and Terahertz Intensities of Hydrogen- and Halogen-Bonding Systems"

15:00-15:40 **Coffee Break**

15:40-17:20 **Invited Lecture n** (Chair: Suehiro Iwata)

15:40 On-1 **Masayoshi Takayanagi**
Nagoya University, Japan
"Multiple oxygen entry pathways in T-state human hemoglobin revealed by ensemble MD simulation"

16:00 On-2 **Martin Srnec**
Institute of Organic Chemistry and Biochemistry, Academy of Science of the Czech Republic
"Elucidation of the Fe^{IV}=O intermediate in the catalytic cycle of Halogenase: Chlorination versus Hydroxylation Selectivity"

16:20 On-3 **Mitsutaka Okumura**
Osaka University, Japan
"Theoretical Investigation for the Catalytic Activities of Au Cluster Catalysts"

16:40 On-4 **Jaroslav Burda (cannot attend)**
Charles University, Czech Republic
"Reaction Mechanism of Ru(II) Piano-Stool Complexes; Umbrella Sampling QM/MM MD Study"

changed to **Masahiko Hada**
Tokyo Metropolitan University, Japan
"Two-Component Relativistic NMR Theory and Quantum-Chemical Analyses of Pt-and Pb-NMR Chemical shifts"

17:00 On-5 **Kazunari Yoshizawa**
Kyushu University, Japan
"Orbital Views of Electron Transport in Molecules"

19:00-21:00 **Banquet (Hotel Nikko Nara, 4F room Hiten)**

Friday, Dec 6

9:00-16:00 **Excursion (Nara Park)**

Poster I, Dec 3

Invited Poster, Ia, Hirayama Hall, 15:00 - 16:40

PIa-01 **Development and parallelization of DC-DFTB method aimed at large scale molecular dynamics**
Hiroaki Nishizawa[1,2], Hiromi Nakai[2,3,4], and Stephan Irle[5]
[1]*Department of Theoretical and Computational Molecular Science, Institute for Molecular Science,* [2]*Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University,* [3]*CREST, Japan Science and Technology Agency,* [4]*ESICB, Kyoto University,* [5]*Department of Chemistry, Graduate School of Science, Nagoya University*

PIa-02 **MP2-F12 study of interaction energies of large molecules with K computer**
Yu-ya Ohnishi, Kazuya Ishimura, Seiichiro Ten-no
Graduate School of System Informatics

PIa-03 **Multiple-input parallel RHF calculation for improving SIMD operation efficiency**
Hiroaki Honda,[1,4] Yuichi Inadomi,[2,4] and Jun Maki[3]
[1]*Research Institute for Information Technology, Kyushu University,* [2]*Graduate School of Information Science and Electrical Engineering, Kyushu University,* [3]*Institute of Systems, Information Technologies and Nanotechnologies,* [4]*JST-CREST*

PIa-04 **Essentially exact ground-state calculations of few-electron molecular systems by superpositions of nonorthogonal Slater determinants**
Hidekazu Goto, Akihiko Okimura, and Kikuji Hirose
Department of Precision Science & Technology, Graduate School of Engineering, Osaka University

PIa-05 **Recent progress in quantum chemical density matrix renormalization group methods**
Takeshi Yanai,[1,2] Yuki Kurashige,[1,2] Jakub Chalupský,[1] Masaaki Saitow,[2] Tran Nguyen Lan[2]
[1]*Department of Theoretical and Computational Molecular Science, Institute for Molecular Science,* [2]*The Graduate University for Advanced Studies*

PIa-06 **New Orbital Optimization Approach via Thouless Theorem.**
Ján Šimunek[1] and Jozef Noga[1,2,3]
[1]*Department of Inorganic Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava,* [2]*Institute of Inorganic Chemistry, Slovak Academy of Sciences,* [3]*Computing Centre, Slovak Academy of Sciences*

PIa-07 **Statistical mechanics based on cumulant dynamics**
Yasuteru Shigeta, Takeshi Baba, Hiroyuki Ando, Ryota Nakamura, Taku Takebayashi, Ryohei Kishi, and Masayoshi Nakano
Graduate School of Engineering Science, Osaka University

PIa-08 **Time Evolution of Atomic and Molecular Systems by Rigged QED**
Kazuhide Ichikawa, Masahiro Fukuda, Akitomo Tachibana
Department of Micro Engineering, Kyoto University

PIa-09 **Surface effects on the reactivity of CeO_2 for hydration of cyanopyridine**
Kyoichi Sawabe, Yukio Yoshikawa, and Atsushi Satsuma
Graduate School of Engineering, Nagoya University

PIa-10 **Development of model effective Hamiltonian to study low-lying d−d excited states of $[Fe(bpy)_3]^{2+}$**
Satoru Iuchi and Nobuaki Koga
Graduate School of Information Science, Nagoya University

PIa-11 **Crystal Structure Prediction by using the GRRM method**
Hideo Yamakado,[1] Hiroaki Tokoyama,[1] Yu Sawada,[1] Yoshitomo Kodaya,[1] Satoshi Maeda[2] and Koichi Ohno[3]
[1]*Faculty of Systems Engineering, Wakayama Univ.* [2]*Graduate School of Science, Hokkaido Univ..,* [3]*Institute for Quantum Chemical Exploration; Graduate School of Science, Tohoku Univ.*

PIa-12 Density Functional Study of Selective Binding to Negatively Charged N_2S_2-type Co(III) complex

Hiroaki Wasada[1], Yuko Wasada-Tsutsui[2], Takuma Yano[2], Tomohiko Inomata[2], Yasuhiro Funahashi[2], Tomohiro Ozawa[2], Hideki Masuda[2]

[1]Faculty of Regional Studies, Gifu University, [2]Nagoya Institute of Technology

PIa-13 Unique Spin State of Inverted Sandwich Type Complexes with Hetero Dinuclear Transition Metals Bridged by Dinitrogen Molecule

Masayuki Nakagaki, Shigeyoshi Sakaki

Fukui Institute for Fundamental Chemistry, Kyoto University

PIa-14 Theoretical Study of the TiO_2-TCNX Surface Complex Showing Interfacial Charge-Transfer Transitions

Ryota Jono, and Koichi Yamashita

The University of Tokyo, JST-CREST

PIa-15 Computational Modeling of Protein Functions: Molecular Recognition and Enzymatic Catalysis

Toyokazu Ishida

Nanosystem Research Institute (NRI), National Institute of Advanced Industrial Science and Technology (AIST)

PIa-16 Ion mobility mass spectrometry and MM conformational search of glycopeptides

Michiko Tajiri,[1] Takae Takeuchi,[2] and Yoshinao Wada[1]

[1]Osaka Medical Center and Research Institute for Maternal and Child Health, [2]Nara Women's University

PIa-17 Theoretical Calculations of Electronic Circular Dichroism for Single and Double Helicenes

Mina Ikenosako, Takeharu Kusuki, Yoshito Nakai, Yoshihisa Inoue, and Tadashi Mori

Graduate School of Engineering, Osaka University

PIa-18 Spectroscopy and Dynamics of Molecular Multiply Excited States

Takeshi Odagiri[1] and Noriyuki. Kouchi[2]

[1]Department of Materials and Life Sciences, Sophia University, [2]Department of Chemistry, Tokyo Institute of Technology

PIa-19 Auger decay spectra calculations for some small molecules

Osamu Takahashi,[1] Saya Takaki,[2] Naotake Kunitake,[2] Katsuyoshi Yamasaki[2]

[1]Institute for Sustainable and Development, Hiroshima University, [2]Department of Chemistry, Hiroshima University

PIa-20 A Hybrid CASSCF/MRMP2 Method for the Quantitative Calculations of the Spin–Orbit Term of Zero-Field Splitting Tensors: A Case Study on Halogen-Substituted High-Spin Nitrenes

Kenji Sugisaki,[1] Kazuo Toyota,[1] Kazunobu Sato,[1] Daisuke Shiomi,[1] Masahiro Kitagawa,[2] and Takeji Takui[1]

[1]Department of Chemistry, Graduate School of Science, Osaka City University, [2]Department of System Innovation, Graduate School of Engineering Science, Osaka University

PIa-21 DFT Calculations of the Spin–Orbit Term of Zero-Field Splitting Tensors: An Orbital Region Partitioning for the Analysis of PK-DFT, and Proposal of a Modified QRO Method

Kenji Sugisaki,[1] Kazuo Toyota,[1] Kazunobu Sato,[1] Daisuke Shiomi,[1] Masahiro Kitagawa,[2] and Takeji Takui[1]

[1]Department of Chemistry, Graduate School of Science, Osaka City University, [2]Department of System Innovation, Graduate School of Engineering Science, Osaka University

PIa-22 Transition-Density-Fragment Interaction Combined with Transfer Integral Approach for Excitation-Energy Transfer via Charge-Transfer States

Kazuhiro J. Fujimoto

Department of Computational Science, Kobe University

PIa-23 Electronic excitations of conjugated molecules in vacuum and in solution

Ryoichi Fukuda, and Masahiro Ehara

[1]Institute for Molecular Science and Research Center for Computational Science, [2]Elements Strategy Initiative for Catalysts and Batteries (ESICB) Kyoto University

PIa-24 Efficient algorithm to optimize structures and reaction paths on free energy surface using QM/MM MD simulation

Toshio Asada
Department of Chemistry, Osaka Prefecture University

PIa-25 Analysis and efficient time evolution of real-time TDHF/TDDFT calculation for electron dynamics

Tomoko Akama
Faculty of Science and Technology, Sophia University

PIa-26 Theoretical study on chemical reactions including non-adiabatic electron dynamics under laser fields.

Takehiro Yonehara and Kazuo Takatsuka
The University of Tokyo, TCCI, CMSI,

PIa-27 Theoretical study of magnetism of Mn clusters using general spin orbital DFT

Shusuke Yamanaka, Yasutaka Kitagawa, Takashi Kawakami, Mitsutaka Okumura, Haruki Nakamura, and Kizashi Yamaguchi
[1]Graduate School of Science ,Osaka University, [2]Protein Institute, Osaka University, [3]NanoScience Design Center, Osaka University

PIa-28 Solid State Spectroscopic Properties of New Heterocycles: MS-CASPT and FMO Studies

Yasuhiro Shigemitsu[1,2]
[1]Industrial Technology Centre of Nagasaki, [2]Graduate School of Engineering, Nagasaki University

PIa-29 Quantum Computation of the properties of acrylamide

Yi-De Lin, Yi-Siang Wang and Sheng D. Chao
Institute of Applied Mechanics, National Taiwan University

PIa-30 Theoretical and UV Spectroscopic Considerations on the Proton-Transfer from Alcohols to Alkyl Pyridinimines

Naoya Iwasaki and Takayuki Suzuki
Department of Green and Sutainable Chemistry, Tokyo Denki University

PIa-31 Essential Coordinates to Describe the Dynamics of Many-atom Systems

Shinnosuke Kawai,[1] Hiroshi Teramoto,[2] and Tamiki Komatsuzaki[2]
[1]Department of Chemistry, Faculty of Science, Shizuoka University, [2]Research Institute for Electronic Science, Hokkaido University

PIa-32 Molecular Design for Light-Emitting Molecules

Tohru Sato
[1]Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, [2]Unit of Elements Strategy Initiative for Catalysts & Batteries, Kyoto University

PIa-33 Inner-shell ionized and excited states of carbon oxide and carbon sulfide compounds: open-shell reference (OR)-SAC/SAC-CI theoretical studies

Yasushi Honda[1] and Hiroshi Nakatsuji[2,3]
[1]West-Japan Office, HPC Systems Inc. [2]Quantum Chemistry Research Institute (QCRI), JST-CREST, [3]Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University

PIa-34 Laser-Polarization Effects on Coherent Vibronic Excitationof Molecules with Quasi-Degenerate Electronic States

Manabu Kanno, Yukari Ono, Hirohiko Kono, and Yuichi Fujimura
Department of Chemistry, Graduate School of Science,Tohoku University

PIa-35 Protein Simulations by Generalized-Ensemble Molecular Dynamics Method

Yoshiharu Mori, Satoru G. Itoh, Hisashi Okumura
[1]Research Center for Computational Science, Institute for Molecular Science, [2]Department of Structural Molecular Science, The Graduate University for Advanced Studies

PIa-36 Theoretical studies on the electronic state of helical conformation with π conjugated systems

Azusa Muraoka
Department of Physics, Meiji University,

PIa-37 Development of optimal control simulation with nonlinear interactions and its applications
Yukiyoshi Ohtsuki, Masataka Yoshida, Kaoru Nakashima, Katsuhiro Nakajima, Hiroya Abe
Department of Chemistry, Graduate School of Science, Tohoku Uiversity

PIa-38 Exploring Theoretical Models for Water
Shigenori Tanaka
Graduate School of System Informatics, Kobe University

PIa-39 Molecular Informatics by Electronic-Structure Simulations
Manabu Sugimoto
Department of Applied Chemistry and Biochemistry, Kumamoto University and JST-CREST

PIa-40 A Theoretical Study on Proton-Conduction Mechanism for Perovskite-Type Compounds
Taku Onishi[1,2], and Trygve Helgaker[2]
Department of Chemistry for Materials, and The Center of Ultimate Technology on nano-Electronics, Mie University, [2]Centre for Theoretical and Computational Chemistry (CTCC), Department of Chemistry, University of Oslo, Norway

PIa-41 Level Structure of Excited States and Two-Photon Absorption Properties of Cyclic Paraphenylene Compounds
Tomotaka Namikawa, Koji Ohta, Kenji Kamada, Katsuma Matsui, Yasutomo Segawa, and Kenichiro Itami
[1]Research Institute for Ubiquitous Energy Devices, National Institute of Advanced Industrial Science and Technology (AIST), [2]Institute of Transformative Bio-Molecules (WPI-ITbM) & Graduate School of Science, Nagoya University, [3]JST-ERATO, Itami Molecular Nanocarbon Project, Nagoya University

Normal Poster, Ib, Meeting Room A, 15:00 - 16:40

PIb-01 Theoretical study of photoisomerization reaction between cyclohexadiene and hexatriene
Ayumi Ohta, Osamu Kobayashi, Toshimasa Ishida, and Shinkoh Nanbu
Faculty of Science and Technology, Sophia University

PIb-02 Theoretical study of cyclodextrins from gas phase to aqueous solution: intramolecular and intermolecular hydrogen bonding
Dai Akase and Misako Aida
Center for Quantum Life Science and Department of Chemistry, Graduate School of Science, Hiroshima University

PIb-03 Hydration Helmholtz energy of adamantane and halo-substituted adamantanes
Hideo Doi, and Misako Aida
Hiroshima University

PIb-04 Molecular Dynamics Simulation of the Photodesorption of Crystalline and Amorphous CO Ice in Interstellar Space
Marc C. van Hemert,[1] Junko Takahashi,[2] Ewine F. van Dishoeck[3]
[1]Institute of Chemistry, University of Leiden, The Netherlands, [2]Meiji Gakuin University, [3]Leiden Observatory, University of Leiden, The Netherlands

PIb-05 Spontaneous Conformational Change of the C-terminal Region of U1A Suggests a Combined Mechanism of Conformational-selection and Induced-fit in the U1A-RNA Molecular Recognition
Ikuo Kurisaki,[1,2] Masayoshi Takayanagi,[1,2,3] Masataka Nagaoka[1,2]
[1]Graduate School of Information Science, Nagoya University; [2]CREST, JST; [3]Venture Business Laboratory, Nagoya University

PIb-06 Role of acidic proton in the decomposition of NO over dimeric Cu(I) active sites in Cu-ZSM-5 catalyst
P. K. Sajith, Yoshihito Shiota and Kazunari Yoshizawa
Institute for Materials Chemistry and Engineering and International Research Center for Molecular Systems, Kyushu University, Fukuoka 819-0395, Japan

PIb-07 A Study of Microrheology by the Time Dependent Density Functional Theory
Masao Inoue and Akira Yoshimori
Department of Physics, Kyushu University, Fukuoka 812-8581, Japan

PIb-08 Explicit solvent effects on vibrational spectra of glycine: Vibrational frequency analysis using analytical Hessian

Yukichi Kitamura,[1,2] Norio Takenaka,[1,3] Yoshiyuki Koyano,[1] and Masataka Nagaoka[1,3]
[1]Graduate School of Information Science, Nagoya University,[2]Research Fellow of Japan Society for the Promotion of Science (JSPS),[3]ESICB, Kyoto University

PIb-09 A new theoretical approach to find single bond activation pathways on metal cluster: A case study of H_2 dissociation on gold clusters

Min Gao, Satoshi Maeda, Andrey Lyalin, and Tetsuya Taketsugu
Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo, 060-0810, Japan

PIb-10 Methane C–H bond Activation by Iron-Oxo Embedded Graphene: A Density Functional Theory Approach

Sarawoot Impeng,[1,2] Chompunuch Warakulwit,[1,2] Pipat Khongpracha,[1,2] Jumras Limtrakul[1,2] and Masahiro Ehara[3]
[1]Department of Chemistry, and NANOTEC Center for Nanoscale Materials Design for Green Nanotechnology, Kasetsart University, Thailand, [2]Center for Advanced Studies in Nanotechnology and Its Applications in Chemical, Food and Agricultural Industries, Kasetsart University, Thailand, [3]Institute for Molecular Science and Research Center for Computational Science

PIb-11 Impact of intermolecular interaction on the second hyperpolarizability of phenalenyl radical dimer

Kyohei Yoneda, Kotaro Fukuda, Hiroshi Matsui, Yuta Hirosaki, Shota Takamuku, and Masayoshi Nakano
Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University

PIb-12 Systematic exploration of reaction mechanisms for a vinylogous Mannich-type reaction activated by a water molecule: kinetic control vs. thermodynamic control

Ryohei Uematsu, Satoshi Maeda, and Tetsuya Taketsugu
Graduate School of Chemical Sciences and Engineering, Hokkaido University,

PIb-13 Effects of the Silyl Substituent of Diphenylprolinol Silyl Ether in the Organocatalyst-Mediated Asymmetric Reactions: Computational and Experimental Investigations

Tadafumi Uchimaru,[1] Seiji Tsuzuki,[1] Daichi Okamura,[2,3] Tatsuya Yamazaki,[3] Yasuto Ameda,[3] Hiroaki Gotoh,[3] Yujiro Hayashi[2,3]
[1]Nanosystem Research Institute, Advanced Industrial Science and Technology, [2]Department of Chemistry, Graduate School of Science, Tohoku University, [3]Department of Industrial Chemistry, Faculty of Engineering, Tokyo University of Science

PIb-14 Diradical character based design for singlet fission in heteroacene molecules

Soichi Ito and Masayoshi Nakano
Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University

PIb-15 Theoretical evaluation of photostability for Sun Protect molecule in UV energy region

Ryota Shimada,[1] Toshimasa Ishida,[2] Shinkoh Nanbu[1]
[1]Sophia University , [2]Individual

PIb-16 Ground state study of LiX, NaX, KX and RbX (X = Ca, Sr) polar molecules

Geetha Gopakumar,[1,2] Minori Abe,[1,2] Masahiko Hada[1,2] and Masatoshi Kajita[3]
[1]Department of Chemistry, Tokyo Metropolitan University, [2]JST, CREST, [3]National Institute of Information and Communications Technology

PIb-17 A reparametrization approach of the B3LYP functional based on the equilibrium temperature of the spin crossover compounds.

Ahmed Slimani, Xuefang Yu, Koichi Yamashita
Department of Chemical System Engineering, The University of Tokyo

PIb-18 Metal Dependency and Protein Environment Effect on the Optical and Electronic Properties of Metalloporphyrin-Ligand Systems

Mitsumasa Abe, Masami Lintuluoto
Graduate School of Life and Environmental Sciences, Kyoto Prefectural University

PIb-19 Localized vs. Delocalized Ground and Excited States of Mn(III) and Ni(II) Salen Complexes: Theoretical Study of Solvation Effects

Shinji Aono, Masayuki Nakagaki, Shigeyoshi Sakaki
Fukui Institute for Fundamental Chemistry, Kyoto Univ.

PIb-20 Electronic Structure of N_2-bridged lanthanide single-molecule magnet

Yue Chen and Shigeyoshi Sakaki
Fukui Institute for Fundamental Chemistry, Kyoto Unviersity

PIb-21 Large-scale MP2 calculation based on spin-dependent two-component Hamiltonian and divide-and-conquer approach

Masahiko Nakano,[1] Junji Seino,[1] and Hiromi Nakai[1-4]
[1]Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University, [2]Research Institute for Science and Engineering, Waseda University, [3]CREST, Japan Science and Technology Agency, [4]Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University

PIb-22 An *ab initio* study of nuclear volume effects using 2-compornent relativistic method for isotope fractionation

Keisuke Nemoto,[1,3] Minori Abe,[1,3] Junji Seino,[2,3] Masahiko Hada[1,3]
[1]Department of Chemistry, Graduate School of Science and Engineering, Tokyo Metropolitan University, [2]School of advanced science and engineering, Waseda University, [3]JST-CREST

PIb-23 Relativistic corrections for an electron confined by two-dimensional quantum dots

Kyozaburo Takeda[1] and Yasuhiro Tokura[2]
[1]Waseda University, [2]University of Tsukuba

PIb-24 Theoretical study of atomic and molecular systems using electronic stress tensor density and energy density

Hiroo Nozaki, Kazuhide Ichikawa, Akitomo Tachibana
Department of Micro Engineering, Kyoto University

PIb-25 Four-Component Relativistic Occupation Restricted Multi-active Space Self-Consistent Field and its Application to Multireference Perturbation Theory

Satoshi Suzuki, Yoshihiro Watanabe, and Haruyuki Nakano
Department of Chemistry, Graduate School of Sciences, Kyushu University,

PIb-26 A highly scalable multireference configuration interaction theory: DMRG-MRCI

Masaaki Saitow,[1] Yuki Kurashige[2] and Takeshi Yanai[2]
[1]The Graduate University for Advanced Studies, [2]Institute for Molecular Science

PIb-27 DMRG CAS-SI employing flexible nuclear screening spin-orbit approximation

Jakub Chalupský, Yuki Kurashige, and Takeshi Yanai
Department of Theoretical and Computational Molecular Science, Institute for Molecular Science

PIb-28 Chemically intuitive indices for charge-transfer excitation based on SAC-CI and TD-DFT calculations

Masahiro Ehara, Ryoichi Fukuda, Carlo Adamo, and Ilaria Ciofini
Institute for Molecular Science

PIb-29 General Coalescence Conditions for the Exact Wave Functions: Higher-Order Relations for Many-Particle Systems

Yusaku I. Kurokawa, Hiroyuki Nakashima, Hiroshi Nakatsuji
Quantum Chemistry Research Institute

PIb-30 Free Complement Calculations of the Helium atom: Gaussian versus Slater

Johanna Langner[1,2] and Hiroshi Nakatsuji[1]
[1]Quantum Chemistry Research Institute, [2]Universität Leipzig, Fakultät für Chemie und Mineralogie, Germany

PIb-31 Theoretical chiral molecular technology, ChiraSac applied to biological molecules

Tomoo Miyahara and Hiroshi Nakatsuji
Quantum Chemistry Research Institute (QCRI)

Poster II, Dec 4

Invited Poster, IIa, Hirayama Hall, 15:00 - 16:40

PIIa-01 MPI/OpenMP hybrid parallel algorithm of resolution of identity second-order Møller–Plesset perturbation calculation for K computer
Michio Katouda and Tanahito Nakajima
Computational Molecular Science Research Team, RIKEN Advanced Institute for Computational Science

PIIa-02 Massively Parallel Program for Quantum Chemistry Calculations
Kazuya Ishimura
Theoretical and Computational Chemistry Initiative (TCCI), Institute for Molecular Science

PIIa-03 Model Space Quantum Monte Carlo method Hybrid Parallel Implementation and Some Applications
Yuhki Ohtsuka and Seiichiro Ten-no
Graduate School of System informatics, Kobe University

PIIa-04 Time evolution of quantum system based on primary Rigged QED
Masato Senami, Soujiro Takada, and Akitomo Tachibana
Department of Micro Engineering, Kyoto University

PIIa-05 Development of first-principles calculation method under periodic boundary condition for material quantum chemistry
Tomomi Shimazaki, Taichi Kosugi, and Takahito Nakajima
RIKEN, Advanced Institute for Computational Science

PIIa-06 Quantum and semiclassical formulations based on overlap integrals for nonadiabatic dynamics: "Rigorous" surface hopping
Mikiya Fujii
Department of Chemical System Engineering, School of Engineering, The University of Tokyo

PIIa-07 Automated Exploration of Novel Reaction Channels by Massively Controlled GRRM Method
Koichi Ohno
Institute for quantum chemical exploration

PIIa-08 Direct variation of the second-order reduced density matrix: application to two-dimensional Hubbard model
Maho Nakata
Advanced Center for Computing and Communication

PIIa-09 Two-component Relativistic Time-dependent Density Functional Theory: Development and Applications
Yutaka Imamura, Muneaki Kamiya, Takahito Nakajima
RIKEN, Advanced Institute for Computational Science

PIIa-10 Theoretical study on ethanolamine-water complex and ethanolamine dimer using Hamiltonian algorithm
Hiroyuki Teramae,[1] and Yasuko Y. Maruo[2]
[1]*Department of Chemistry, Josai University,* [2]*Department of Environment and Energy, Tohoku Institute of Technology*

PIIa-11 A Density Functional Theory Based Protocol to Compute the Redox Potential for Transition Metal Complexes
Toru Matsui,[1,2] Yasutaka Kitagawa,[1] Yasuteru Shigeta,[3] and Mitsutaka Okumura[1]
[1] *Department of Chemistry, Graduate School of Science, Osaka University,* [2] *Advanced Institute for Computational Science, RIKEN,* [3] *Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University*

PIIa-12 Nano-scale modeling for automotive catalyst
Kei Kuramoto, Koki Hirai, and Tetsuya Ohkawa
University of Hyogo

PIIa-13 Theoretical studies of molecular structures and magnetic properties on polynuclear metal complexes

Yasutaka Kitagawa, Takashi Kawakami, Shusuke Yamanaka and Mitsutaka Okumura
Graduate School of Science, Osaka University, JST-CREST,

PIIa-14 Theoretical Study on Aqueous Lanthanide-Catalyzed Mukaiyama-Aldol Reaction

Miho Hatanaka and Keiji Morokuma
Fukui Institute for Fundamental Chemistry Kyoto University

PIIa-15 Predicting Free Energies of Complexation of Transition Metal-Ions with Small Ligands from the First Principles

Ondrej Gutten[1], Lubomir Rulišek[1]
[1]Institute of Organic Chemistry and Biochemistry, AS CR

PIIa-16 Theoretical study of local and nonlocal molecular interactions in secondary structures

Yu Takano and Haruki Nakamura
Institute for Protein Research, Osaka University,

PIIa-17 Theoretical study for excited states of firefly-bioluminescence-related molecules

Miyabi Hiyama, Kenta Yamada, Toshimitsu Mochizuki, Hidefumi Akiyama, Nobuaki Koga
[1]The Institute for Solid State Physics, The University of Tokyo, [2]Fukui Institute for Fundamental Chemistry, Kyoto University, [3]Graduate School of Information Science, Nagoya University

PIIa-18 Correlation between experimental and theoretical electric circular dichroism spectra of biomolecules in the vacuum ultraviolet region

Masahito Tanaka[1], Yasuhiro Gunji[2], and Kazumichi Nakagawa[3]
[1]National Institute of Advanced Industrial Science and Technology (AIST), [2]Graduate School of Science and Technology, Tokai University, [3] Graduate School of Human Development and Environment, Kobe University

PIIa-19 Understanding IR spectra of perfluorinated sulfonic acid ionomer membranes

Makoto Yamaguchi, and Akihiro Ohira
Fuel Cell Cutting Edge Research Center (FC-Cubic)

PIIa-20 Theoretical calculations of zero-field splitting parameter *D* for single molecular magnets

Takashi Kawakami, Keiji Kinoshita, Shohei Yoshimura, Yasutaka Kitagawa, Shusuke Yamanaka, Kizashi Yamaguchi, Mitsutaka Okumura
Department of Chemistry, Graduate School of Science, OSAKA University

PIIa-21 Ab initio Calculation of Zero-Field Splitting Tensor in Organic Compounds

Kazuo Toyota, Kazunobu Sato, Daisuke Shiomi, and Takeji Takui
Department of Chemistry, Graduate School of Science, Osaka City University

PIIa-22 Free energy calculations for chemical reactions in condensed phase with massively parallel QM/MM simulations

Hideaki Takahashi, Yuji Miki, Akihiro Morita
Department of Chemistry, Graduate School of Science, Tohoku University

PIIa-23 Theoretical Simple Estimation and Accurate Evaluation of Local Aromaticity for Polycyclic Conjugated Hydrocarbons

Shogo Sakai and Yuuki Kita
Department of Chemistry and Biomolecular Science, Faculty of Engineering, Gifu University

PIIa-24 Theoretical study on the electronic structures and optical response properties of one-dimensional open-shell oligomers involving five-membered rings

Ryohei Kishi, Hideki Uenaka, Yusuke Murata, Keisuke Morita, Michika Saito, Yasuteru Shigeta, and Masayoshi Nakano
Graduate School of Engineering Science, Osaka University

PIIa-25 Novel [2+1] Reaction Pathway for Disilacyclobutenes with Acetylene

Yoshihiro Hayashi, Takafumi Natsumeda, Shun Otsu, Ryo Yamada, and Susumu Kawauchi
Department of Organic and Polymeric Materials, Tokyo Institute of Technology

PIIa-26 Ab Initio Molecular Orbital Studies of Aromatic Excimers and Excited States of Paracyclophanes.
Soichi Shirai,[1,2] Suehiro Iwata,[3] Yoshifumi Maegawa,[1,2] Takao Tani[1,2] and Shinji Inagaki[1,2]
[1]Toyota Central R&D Labs., Inc., [2]JST-CREST, [3]Toyota Physical & Chemical Research Institute

PIIa-27 Theoretical investigation of the binding of a positron to vibrational excited states of polyatomic molecules with quantum Monte Carlo method
Yukiumi Kita and Masanori Tachikawa
Quantum Chemistry Division, Yokohama City University

PIIa-28 Computational Study for Intra-molecular Tunnel Couplings: Bridge-mediated Excitation Energy Transfer / Conformational Exchange of Molecules
Tsutomu Kawatsu,[1,2] Jun-ya Hasegawa,[3] and Shinichi Miura[2]
[1] Institute for Molecular Science, [2] Graduate School of Natural Science and Technology, Kanazawa University, [3]Catalysis Research Center, Hokkaido University

PIIa-29 Acute Aquatic Toxicity Considering the Reactivity of alpha, beta-Unsaturated Carbonyl Compounds
Ayako Furuhama, Yasunobu Aoki, Hiroaki Shiraishi
Center for Environmental Risk Research, National Institute for Environmental Studies (NIES)

PIIa-30 Theoretical Crystal Structure Prediction with the Aid of High Performance Computing
Shigeaki Obata, Mitsuaki Sato and Hitoshi Goto
Information and Computer Science, Toyohashi University of Technology

PIIa-31 Difference Density Matrix Analysis: Application to Substituent Effects and Intermolecular Interactions
Daisuke Yamaki
Research Organization for Information Science and Technology (RIST)

PIIa-32 Quantum interference effect observed in the angular momentum polarization and the branching ratio of photofragments of simple molecules
Takahide Matsuoka, Tomoya Ikezaki, Yusuke Ohta, and Satoshi Yabushita
Department of Chemistry, Faculty of Science and Technology, Keio University

PIIa-33 DFT-MD Studies on Redox Reactions on Solid-Solution Interfaces in Battery and Solar Cell
Y. Tateyama,[1,2,3] K. Sodeyama,[1,3] K. Ushirogata,[4] Y. Okuno,[4] M. Sumita[1]
[1]International Center for Materials Nanoarchitectonics (WPI MANA), National Institute for Materials Science (NIMS), [2]PRESTO & CREST, Japan Science and Technology Agency (JST), [3]Elements Strategy Initiative for Catalysts & Batteries (ESICB), Kyoto University, [4]FUJIFILM Corporation

PIIa-34 Towards Accurate Calculation of Free Energies in Gas-Phase and Solution by Quantum Chemistry
Atsushi Ishikawa and Hiromi Nakai
Waseda University, JST-CREST

PIIa-35 Relativistic coupled cluster studies for electron's electric dipole moment arising from Charge-Parity violation
M. Abe,[1,2] G. Gopakumar,[1,2] B. P. Das,[3] H. Tatewaki,[4] M. Hada,[1, 2] and D. Mukherjee[5]
[1]Department of Chemistry, Tokyo Metropolitan University, [2]JST, CREST, [3]Indian Institute of Astrophysics, [4]Graduate School of Natural Sciences, Nagoya City University, [5]Raman Centre for Atomic, Molecular and Optical Sciences, Indian Association for the Cultivation of Science

PIIa-36 Theoretical Study of the Substituent and Solvent Effects on Azide-Tetrazole Equilibrium of 2-Azido-1,3-benzothiazoles
cannot attend
Walid M. I. Hassan, Sabry El-Taher and Mahmoud A. Noamaan
Chemistry Department, Faculty of Science, Cairo University

PIIa-37 A new perspective of solvation theory
Hirofumi Sato
Department of Molecular Engineering, Kyoto University

PIIa-38 **The ring deformation of hydrogen maleate anion: A path integral molecular dynamics study**
Yukio Kawashima[1] and Masanori Tachikawa[2]
[1]*RIKEN AICS,* [2]*Quantum Chemistry Division, Graduate School of Science, Graduate School of Nanobioscience, Yokohama City University*

PIIa-39 **Cooperative Roles of Charge-Transfer and Dispersion Terms in Hydrogen Bonds of Water Clusters**
Suehiro Iwata
[1]*Department of Chemistry, Faculty of Science and Technology, Keio University,* [2]*Toyota Physical and Chemical Research Institute, and* [3]*Institute for Molecular Science*

PIIa-40 **BINDING $Pt^{IV}(DACH)Cl_4$ TO GMP AND FOLLOWED-UP REDUCTION OF PLATINUM LEADED TO FORMATION OF $Pt^{II}(DACH)Cl_2$**
F. Šebesta, J.V. Burda
Faculty of Mathematics and Physics, Charles University in Prague

PIIa-41 **Non-Adiabatic Molecular Dynamics with FOMO-CAS-CI method**
Lukáš Šištík and Petr Slavíček
[1]*Department of Physical Chemistry, Institute of Chemical Technology,* [2]*J. Heyrovský Institute of Physical Chemistry*

Normal Poster, IIb, Meeting Room A, 15:00 - 16:40

PIIb-01 **2-Chlorobutane racemization process in DMF solution: Application of hybrid MC/MD reaction method**
Yuichi Suzuki,[1] Takuya Okamoto,[1] Norio Takenaka[1,2] and Masataka Nagaoka[1,2]
[1]*Graduate School of Information Science, Nagoya University,* [2]*ESICB, Kyouto University*

PIIb-02 ***Ab Initio* SemiClassical Molecular Dynamic (AI-SCMD) with ZN-TSH approach --- Photodissociation process for Hydrogen Sulfide**
Tatsuhiro Murakami[1], Yoshiaki Teranishi[2], Alexey Kondorskiy[3], Hiroki Nakamura[4] and Shinkoh Nanbu[1]
[1]*Faculty of Science & Technology, Sophia Univ.,* [2]*Inst. of Physics, National Chiao Tung Univ.,Taiwan,* [3]*P. N. Lebedev Physical Inst., and Moscow Institute of Physics and Technology, Russia,* [4]*Inst. of Molecular Science, National Chiao Tung Univ.,Taiwan*

PIIb-03 **Adsorption states of NO molecule on stepped and kinked Pt(111) surfaces studied by DFT simulations**
Satoshi Makihara, Daisuke Mimura, Kouji Inagaki, Yoshitada Morikawa
Graduate School of Engineering, Osaka University

PIIb-04 **Computational Mutation Analysis of Diol Dehydratase in Glycerol Dehydration**
Kazuki Doitomi,[1] Takashi Kamachi,[1] Tetsuo Toraya[2] and Kazunari Yoshizawa[1]
[1]*Institute for Materials Chemistry and Engneering, Kyushu University,* [2]*Graduate School of Natural and Technology, Okayama University*

PIIb-05 **Double-QM/MM Method for Donor-Acceptor Electron Transfer Studies with Solvent Reorganization**
Zdeněk Futera,[1,2] Keitaro Sodeyama,[2,3] Jaroslav V. Burda[4], Yoshitaka Tateyama[2,3,5]
[1]*Keio University,* [2]*International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science (NIMS),* [3]*ESICB, Kyoto University,* [4]*Charles University in Prague, Czech Republic,* [5]*PRESTO and CREST, Japan Science and Technology Agency (JST)*

PIIb-06 **Application of Ewald Sum for ONIOM method**
Osamu Kobayashi and Nanbu Shinkoh
Department of Materials and Life Sciences, Faculty for Science and Engineering, Sophia University,

PIIb-07 **3D-RISM-SCFAnalysis of the SolventEffect on the ElectronicStructures of Merocyanines**
Yuichi Tanaka, Norio Yoshida, and Haruyuki Nakano
Department of Chemistry, Graduate School of Sciences, Kyushu University,

PIIb-08 **Electrolyte-Dependent Characteristics of the Solid Electrolyte Interphase Film Formation in the Lithium-Ion Batteries**
Norio Takenaka,[1,2] Yuichi Suzuki,[1] Hirofumi Sakai[1] and Masataka Nagaoka[1,2]
[1]*Graduate School of Information Science, Nagoya University, 2ESICB, Kyoto University*

PIIb-09 Intramolecular Electron Transfer in Polar Solvents Calculated by Constrained Density Functional Theory
Satoshi Muraoka and Kenji Morihashi
University of Tsukuba

PIIb-10 Synthesis of Antimalarial of 1,10-Phenanthrolinium Bromide Derivatives from Clove and Wintergreen Oils
Dhina Fitriastuti, Muhammad Idham Darussalam Mardjan, Jumina and Mustofa
Department of Chemistry, Universitas Gadjah Mada, Indonesia

PIIb-11 The oxidative addition of chlorobenzene on bimetallic Au/Pd catalysts: An DFT study
Bundet Boekfau[1,2] Masahiro Ehara,[1] Jumras Limtrakul,[2] Raghu Nath Dhital[1] and Hidehiro Sakurai[1]
[1]Research Center for Computational Science, Institute for Molecular Science, [2]Department of Chemistry, and NANOTEC Center for Nanoscale Materials Design for Green Nanotechnology, Kasetsart University, Thailand.

PIIb-12 Theoretical investigation on poly-*para*phenylenevinylene (PPV) charge transfer process
Koharu Aikawa, and Kenji Morihashi
Graduate School of Pure and Applied Sciences, University of Tsukuba,

PIIb-13 First-principles Calculation of Suzuki-Miyaura Cross Coupling Reaction by Palladium Catalyst
Daisuke Mimura,[1] Atuya Takeda,[1] Susumu Yanagisawa,[2] Kouji Inagaki,[1] Yoshitada Morikawa[1] and Takashi Ikeda[3]
[1]Department of Precision Science and Technology, Graduate School of Engineering, Osaka University, [2]Department of Physics and Earth Sciences, Faculty of Science, University of the Ryukyus, [3]Japan Atomic Energy Agency

PIIb-14 First-principle simulations for matrix-isolation vibrational spectra of noble gas compounds: applications to HXeCl and XeBeO
Keisuke Niimi, Akira Nakayama, Yuriko Ono, Tetsuya Taketsugu
Graduate School of Chemical Sciences and Engineering, Hokkaido University,

PIIb-15 Low-temperature Excess Heat Capacity of Potassium Germanate Glasses
Seiichi Mamiya
Graduate School of Pure and Applied Sciences, University of Tsukuba

PIIb-16 Effect of the donor-π-donor type charge distribution on the second hyperpolarizabilities of open-shell singlet systems – *para*-quinodimethane with point charge model
Kotaro Fukuda and Masayoshi Nakano
Graduate School of Engineering Science, Osaka University,

PIIb-17 Computational Molecular Spectroscopy of ZnOH: Comparison with FeOH and CsOH
Umpei Nagashima,[1] Tsuneo Hirano[1,2]
[1]Nanosystem Research Institute (NRI), National Institute of Advanced Industrial Science and Technology (AIST), [2]Ochanomizu University

PIIb-18 A SAC-CI study of the electronic excitation spectra of the radical anions and cations of azobenzene, stilbene, and benzalaniline
Yung-Ching Chou[1,2] and Hiroshi Nakatsuji[3]
[1]Department of Applied Physics and Chemistry,University of Taipei, Taiwan, [2]short-term research in Quantum Chemistry Research Institute, [3]Quantum Chemistry Research Institute

PIIb-19 Theoretical study of the bimetal effect for CO adsorption at Ag islands on Ni(111)
Yuji Mahara, Junya Ohyama, Kyoichi Sawabe, Atsushi Satsuma
Graduate School of Engineering, Nagoya University

PIIb-20 First-principles study of fast Na diffusion in Na3P
Xuefang Yu, Giacomo Giorgi, Hiroshi Ushiyama, and Koichi Yamashita
Department of Chemica; System Engineering, School of Engineer, The University of Japan

PIIb-21 The role of the inorganic cation MA ($CH_3NH_3^+$) in pseudocubic 3D $MAPbI_3$ organic-inorganic perovskites
Giacomo Giorgi, Jun-Ichi Fujisawa, Hiroshi Segawa, Koichi Yamashita
The University of Tokyo

PIIb-22 DFT Probe on Electronic and Bonding Parameters of *n*NHC and *a*NHC Palladium Complex

N. Radhika,[1] G.Velmurugan,[2] P. Venuvanalingam[2] and M. Hada[1]
[1]Department of Chemistry, Graduate School of Science and Engineering, Tokyo Metropolitan University,, [2]School of Chemistry, Bharathidasan University, Tiruchirappallli , India

PIIb-23 Efficient geometry optimization using accurate two-component relativistic Hamiltonian with local unitary transformation scheme

Yuya Nakajima,[1] Junji Seino,[1] and Hiromi Nakai[1-4]
[1]Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University, [2]Research Institute for Science and Engineering, Waseda University, [3]CREST, Japan Science and Technology Agency, [4]Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University

PIIb-24 Diagonal Born-Oppenheimer Correction based on Relativistic Hamiltonians

Yuji Imafuku,[1,2] Minori Abe,[1,2] Michael.W.Schmidt,[3] Terutaka Yoshizawa,[1,2] Masahiko Hada[1,2]
[1]Department of Chemistry, Graduate School of Science and Engineering, Tokyo Metropolitan University, [2]JST-CREST, [3]Iowa State University

PIIb-25 Accuracy of the two-component methods in the relativistic molecular orbital theory

Nobuki Inoue, Satoshi Suzuki, Yoshihiro Watanabe, and Haruyuki Nakano
Department of Chemistry, Graduate School of Sciences, Kyushu University

PIIb-26 Time Evolution Simulation of Electronic Spin Based on Quantum Electrodynamics

Masahiro Fukuda, Kazuhide Ichikawaand Akitomo Tachibana
Department of Micro Engineering, Kyoto University,

PIIb-27 Toward reliable prediction of hyperfine coupling constants using *ab initio* density matrix renormalization group method: diatomic π−radicals as test cases

Tran Nguyen Lan,[1] Yuki Kurashige,[1,2] and Takeshi Yanai[1,2]
[1]The Graduate University for Advanced Studies, [2]Department of Theoretical and Computational Molecular Science, Institute for Molecular Science

PIIb-28 A New Diagrammatic Interpretation of Fitzgerald-Lorentz Contraction in Special Relativity

Shigeru Obara
Department of Chemistry, Kushiro Campus, Hokkaido University of Education

PIIb-29 Efficient antisymmetrization theory for accurate molecular wave functions: *i*Exg theory

Hiroshi Nakatsuji and Hiroyuki Nakashima
Quantum Chemistry Research Institute

PIIb-30 Determinant-based antisymmetrization theory for the partially correlated wave functions: Nk algorithm

Hiroyuki Nakashima and Hiroshi Nakatsuji
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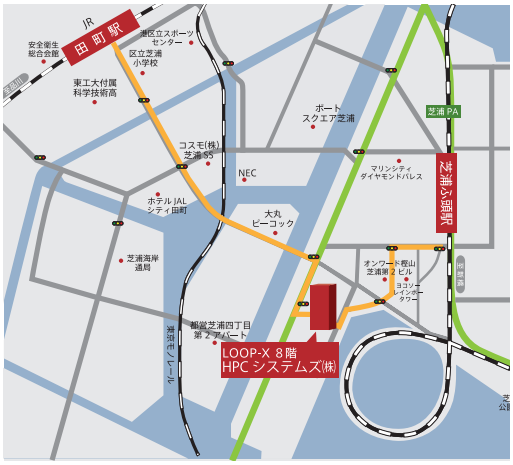

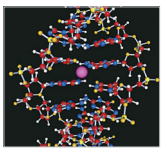
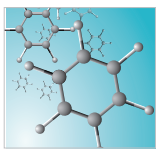

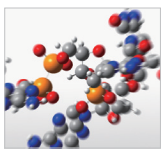
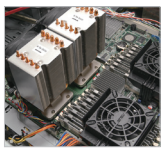

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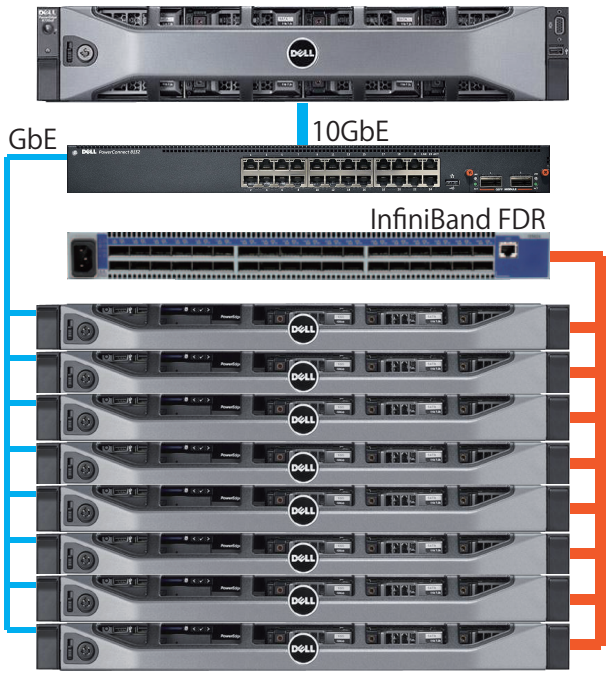

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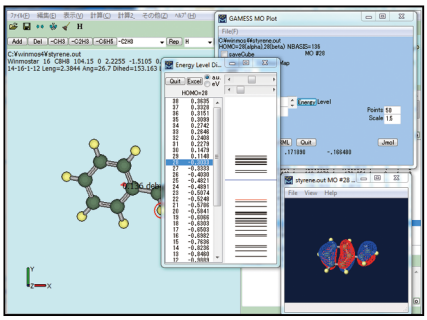
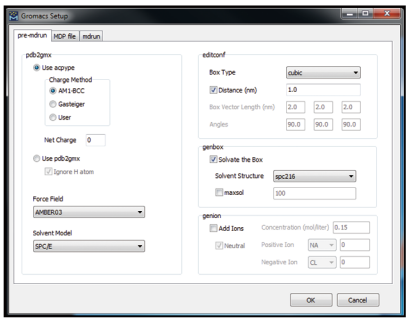
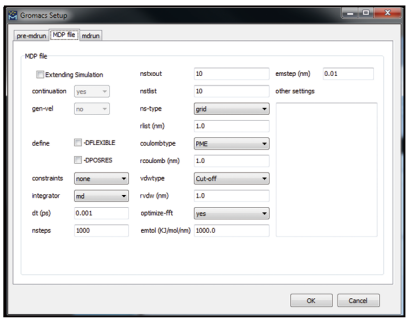
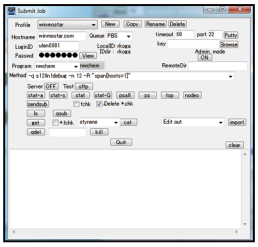
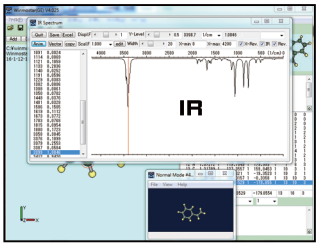

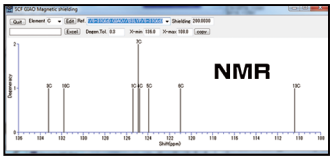

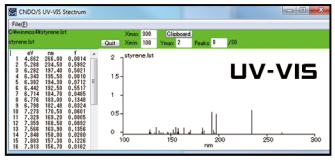

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